3. Intensity of X-rays diffraction

Contents

When performing crystal structure analysis, two main information are obtained:

- The first aspect is the diffraction direction, which is the θ angle. The direction of diffraction reflects the size and shape factor of the unit cell, which can be described by the Bragg equation (Chapter 2).

- The second aspect is the diffraction intensity. The type of atoms inside the substance and the position in the unit cell are reflected in the diffraction results, which are expressed as the intensity of the diffraction line. The Bragg equation cannot describe the intensity problem.

3.1 Formation of phases in polycrystalline diffraction patterns

Take the powder (Debye-Scherrer) method as an example. This method irradiates polycrystalline samples with monochromatic X-rays and records them with strip films. The crystal planes (***d***) satisfying the Bragg equation in the microcrystal are arranged in space as a conical surface with the incident ray as the axis and 2θ as the apex angle; the diffraction lines form a conical surface with a vertex angle of 4θ, see Figure 1.

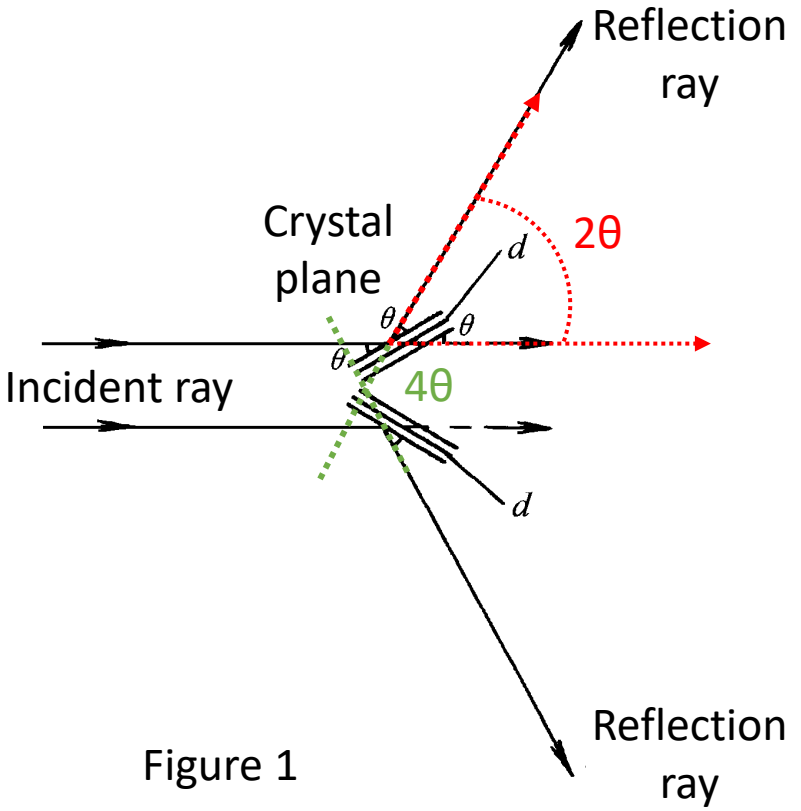
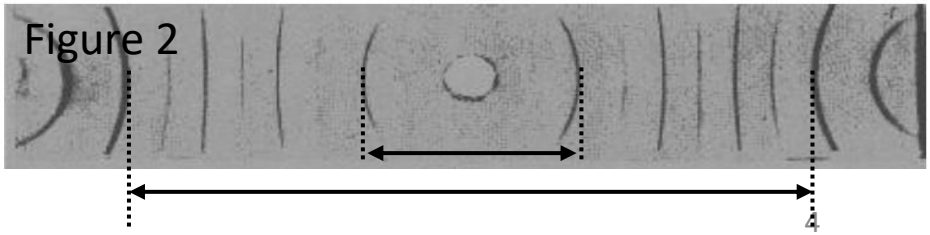


Figure 1

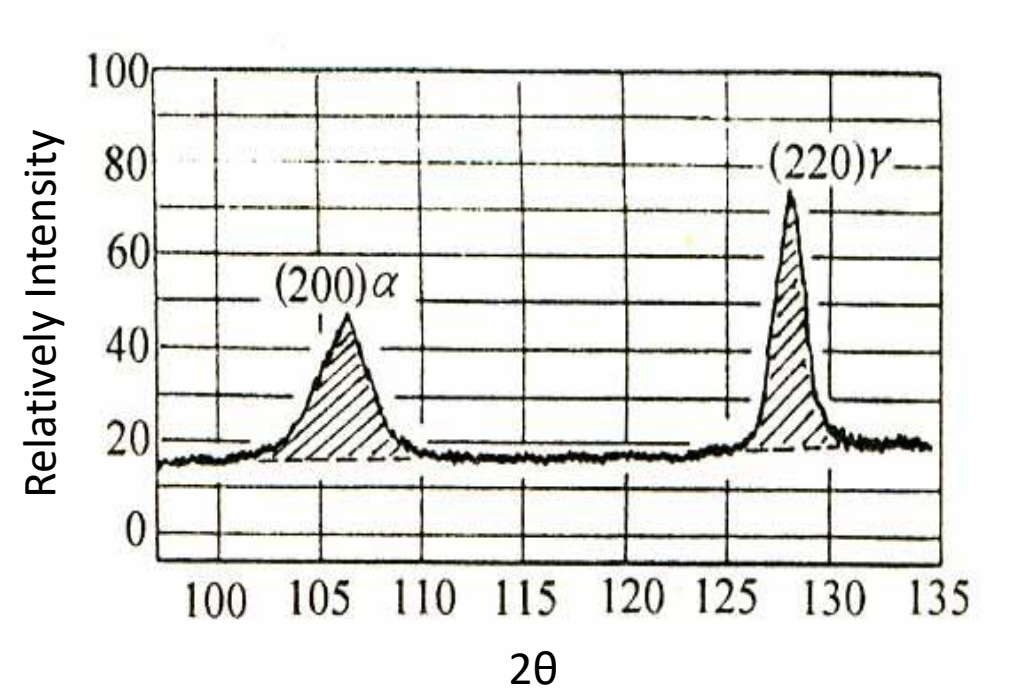
- Crystal planes with different interplanar spacing ***d*** in microcrystals produce different vertex angles 4θ of the diffraction cone.
- When 4θ < 180°, it is a reflection cone, and when 4θ > 180°, , it is a back-reflection cone.
- The recorded diffraction pattern is shown in Figure 2. The diffraction direction determines the position of the diffraction line, and the diffraction intensity determines the brightness of the diffraction line.



3.1 Formation of phases in polycrystalline diffraction patterns

The intensity of X-ray diffraction reflects the height of the diffraction peak on the diffractometer (or the integrated intensity - the area surrounded by the outline of the diffraction peak). It is reflected in the darkness on the film.

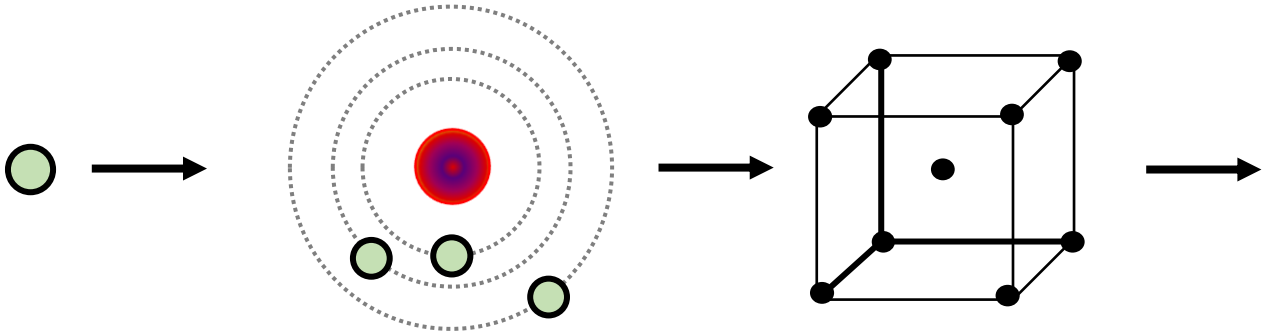
Normally, it is the number of X-ray photons passing through a unit area perpendicular to the diffraction direction per unit time. But this absolute intensity is difficult to measure and has no practical significance. Usually shown in relative intensity.



3.2 X-ray Scattering and Structure Factor of Unit Cell

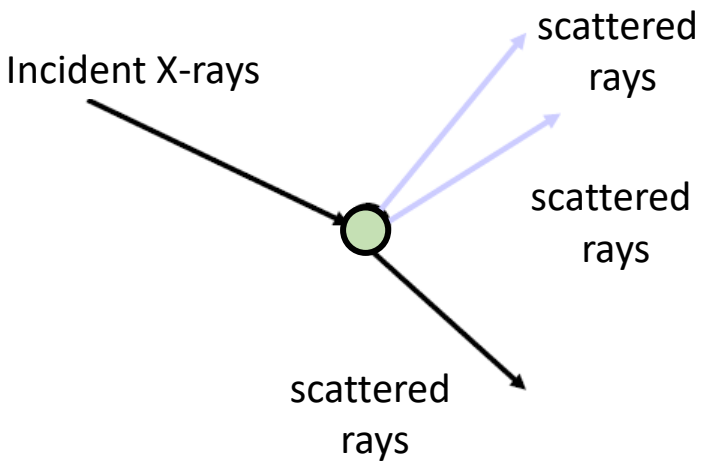
X-ray diffraction intensity

an electron an atom a unit cell powder polycrystalline



3.2 X-ray Scattering and Structure Factor of Unit Cell

X-ray scattering by an electron (**1.5**)



Thomson formula for X-ray scattering by an electron.

$$I_e = \frac{I_0}{R^2}\left(\frac{\mu_0}{4\pi}\right)^2\left(\frac{e^2}{mc}\right)^2\frac{1+\cos^2 2\theta}{2} = \frac{I_0}{R^2} f_e^{\,2}\frac{1+\cos^2 2\theta}{2}$$

- The intensity of the scattered ray of an electron is very weak, about one hundred thousandth of the intensity of the incident ray.

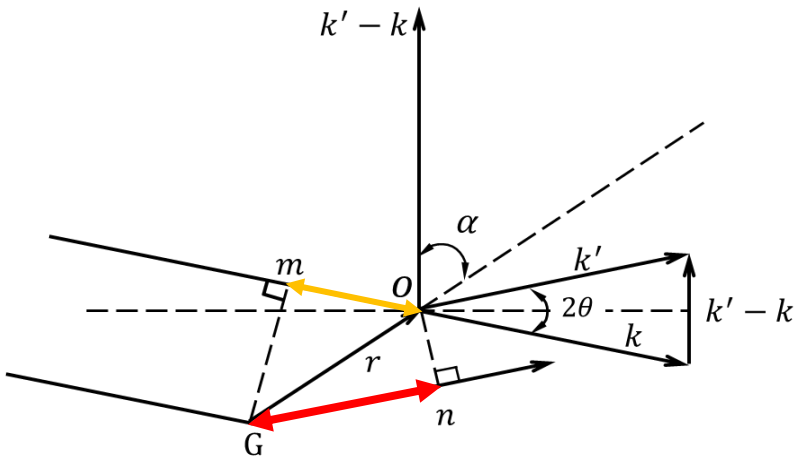
- When 2θ = 0, the intensity of scattered rays is the largest. When 2θ is equal to other angles, the intensity will decrease.

- After a beam of unpolarized X-rays is scattered by electrons, its scattering intensity becomes different in all directions in space and is polarized. The degree of polarization depends on the 2θ angle.

$$\frac{1+(\cos 2\theta)^2}{2}$$ Polarization factor

3.2 X-ray Scattering and Structure Factor of Unit Cell

X-ray scattering by an atom (**1.5**)



- Displacement difference (δ):

  δ = ***Gn*** - ***Om***

- Phase difference (ϕ):

  $\phi=(Gn-Om)2\pi/\lambda$
  $=r\,(S-S_0)\,2\pi/\lambda$
  $=(r2\sin\theta\cos\alpha)\,2\pi/\lambda$
  $=((4\pi\sin\theta)/\,\lambda)r\cos\alpha$
  $=Kr\cos\alpha$

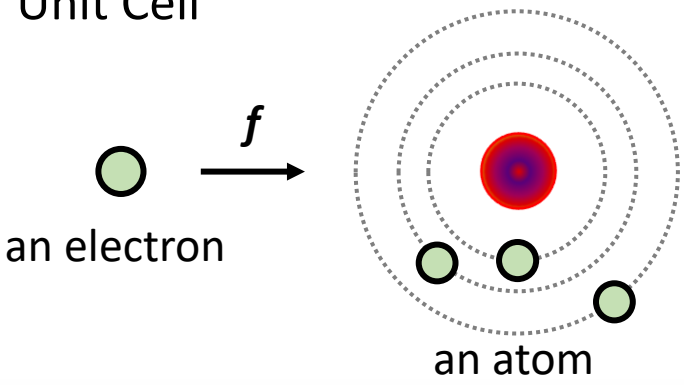
1. The intensity of the scattered waves from an atom should be equal to the sum of the scattered waves from all the electrons in the atom.
2. In order to evaluate the atomic scattering ability, the coefficient ***f*** is introduced, which is called the atomic scattering factor.
3. It is the result of the of all electron scattering waves in the atom after taking into account the phase difference of each electron scattering wave.
4. Numerically, it is expressed as the ratio of the amplitude or intensity of an atomic scattered wave to an electron scattered wave.

3.2 X-ray Scattering and Structure Factor of Unit Cell

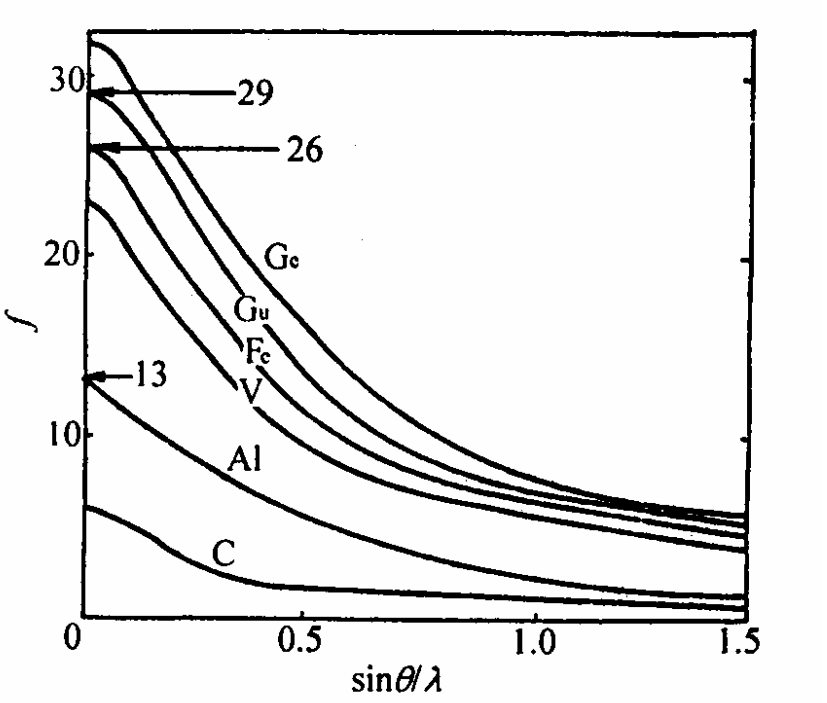
X-ray scattering by an atom (**1.5**)

Atomic scattering factor:

$$f = \frac{A_a}{A_e} = \left(\frac{I_a}{I_e}\right)^{\frac{1}{2}}$$



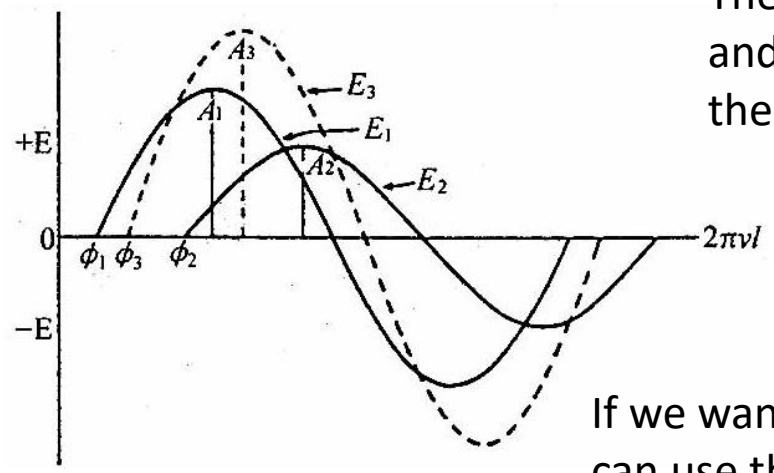
1. The atomic scattering factor can be understood as the scattering wave amplitude of an atom measured in units of an electron scattering wave amplitude.
2. Reflects the scattering rate when an atom scatters X-rays in a certain direction.



Sin* θ / λ** decreases, ***f increases

3.2 X-ray Scattering and Structure Factor of Unit Cell

X-ray scattering by a unit cell



The two wavelengths are the same but different in phase and amplitude. Their wave function can be expressed by the following formula:

$$E_1 = A_1 \sin(2\pi\nu t - \phi_1)$$

$$E_2 = A_2 \sin(2\pi\nu t - \phi_2)$$

If we want to know the superposition of these two waves, we can use the complex number method to perform analytical operations.

1. The wave function in complex exponential form:

$$Ae^{i\phi} = A\cos\phi + Ai\sin\phi$$

2. The sum of multiple vectors can be written as:

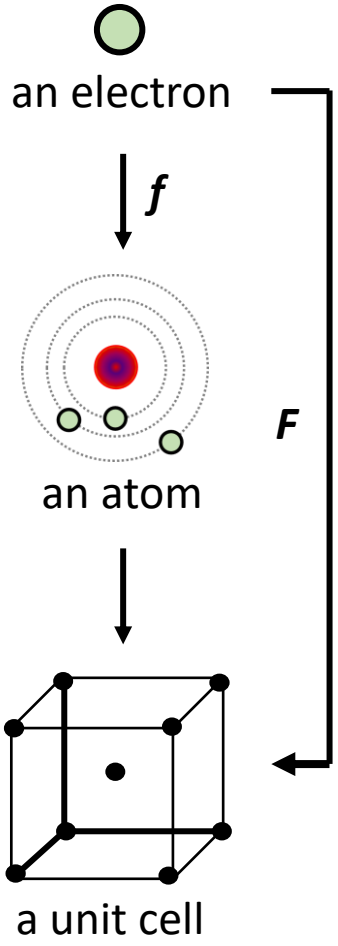
$$\sum Ae^{i\phi} = \sum (Acon\phi + iA\sin\phi)$$

3. The intensity of a wave is proportional to the square of its amplitude:

$$I \propto \left|Ae^{i\phi}\right|^2 = Ae^{i\phi}Ae^{-i\phi} = A^2$$

3.2 X-ray Scattering and Structure Factor of Unit Cell

X-ray scattering by a unit cell



There are m atoms in a unit cell, and the amplitude and orientation of the scattered waves of each atom are different.

The amplitude A_b of the constructive wave of coherent scattered waves from all atoms in the unit cell is:

$$A_b = A_e\left(f_1 e^{i\phi_1} + f_2 e^{i\phi_2} + \cdots + f_m e^{i\phi_n}\right)$$

$$= A_e \sum_{j=1}^{m} f_j e^{i\phi_j}$$

$$F = \frac{A_b}{A_e} = \sum_{j=1}^{m} f_j e^{i\phi_j}$$

Structure factor

3.2 X-ray Scattering and Structure Factor of Unit Cell

X-ray scattering by a unit cell

The phase of the diffracted wave is related to the diffraction plane and the position of the atoms.

$$\phi = 2\pi(Hu + Kv + Lw)$$

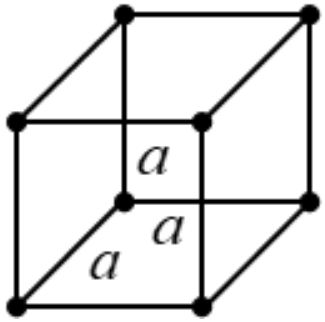
$$F_{HKL} = \sum_{j=1}^{m} f_j e^{2\pi i(Hu_j + Kv_j + Lw_j)} = \sum_{j=1}^{m} f_j \exp[2\pi i(Hu_j + Kv_j + Lw_j)]$$

Structure factor and systematic extinction

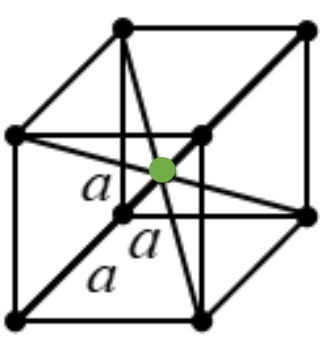
3.2 X-ray Scattering and Structure Factor of Unit Cell

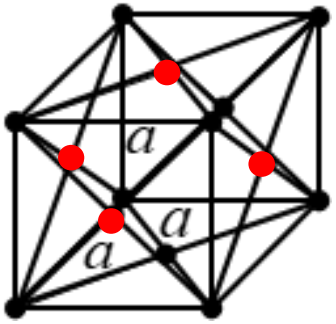
- A simple lattice consists of only one kind of atom. There is only one atom in each unit cell, which is located at the vertex corner of the unit cell. Therefore, the scattering intensity of a simple lattice unit cell is equivalent to the scattering intensity of one atom.

Simple lattice



Complex lattice

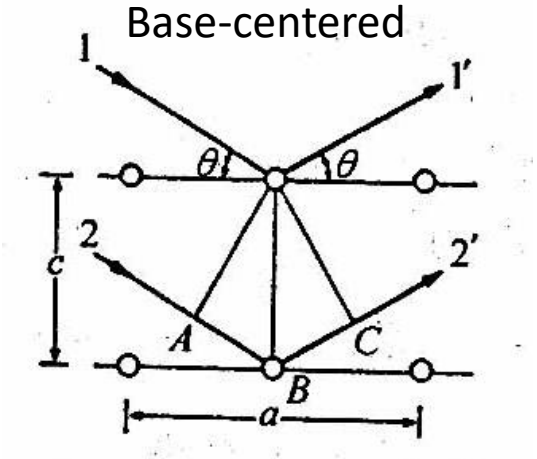




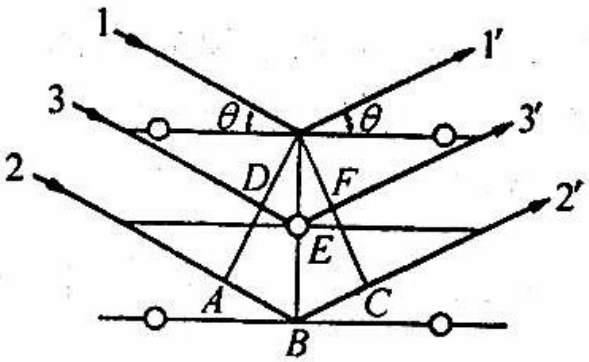
- A unit cell of a complex lattice contains n atoms of the same or different types. In addition to occupying the top corners of the unit cell, they may also be located at the body center, face center or bottom center, so the amplitude of the scattered wave of the complex lattice unit cell is the resultant amplitude of all atomic scattered waves in a unit cell.
- Due to the mutual interference of diffraction lines, the intensity in some directions will be strengthened, and the intensity in some directions will be weakened or even disappear. This phenomenon is customarily called systematic extinction.

3.2 X-ray Scattering and Structure Factor of Unit Cell

Base-centered



Body-centered



- The arrangement of atoms in the crystal is different, which can make the original diffracted beam disappear.
- We call the phenomenon of the disappearance of diffraction lines in certain directions due to different positions of atoms in the crystal or different types of atoms called "system extinction".
- The parameters that quantitatively characterize the arrangement of atoms and the influence of atomic species on X-ray intensity are called structure factors. That is, the influence factor of crystal structure on diffraction intensity.

3.2 X-ray Scattering and Structure Factor of Unit Cell

Derivation of structure factor

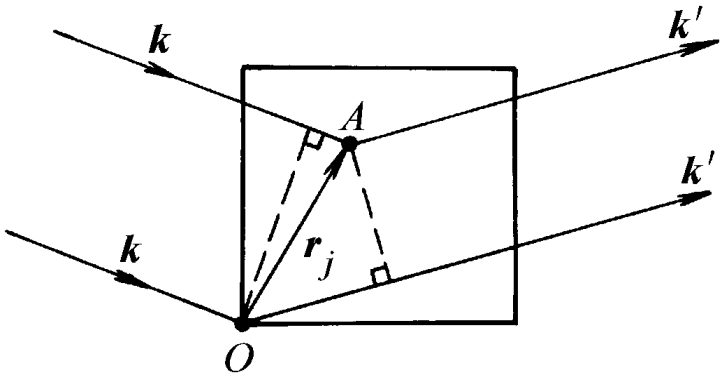
- Taking the unit cell vertex O as the coordinate origin, the position vector of the atom A in the unit cell is:

$$\boldsymbol{r}_j = x_j \boldsymbol{a} + y_j \boldsymbol{b} + z_j \boldsymbol{c}$$

a, ***b***, ***c*** are the basic vectors of the lattice; x_j, y_j, z_j are the coordinates of the A atom.

- The path difference between the scattered waves of A atom and O atom is:

$$\delta_j = \boldsymbol{r}_j \cdot \boldsymbol{k}' - \boldsymbol{r}_j \cdot \boldsymbol{k} = \boldsymbol{r}_j \cdot (\boldsymbol{k}' - \boldsymbol{k})$$



- The corresponding phase difference is:

$$\phi_j = 2\pi(Hx_j + Ky_j + Lz_j)$$

- The superposition of the scattered wave amplitudes of all atoms in the unit cell is the scattered wave amplitude of the unit cell:

$$A_b = A_e \sum_{j=1}^{n} f_j e^{i\phi_j}$$

Atomic scattering factor (***f***):combined amplitude of coherent scattered waves of all electrons in an atom to the amplitude of coherent scattered waves of one electron.

3.2 X-ray Scattering and Structure Factor of Unit Cell

Derivation of structure factor

Introducing a parameter that reflects the scattering ability of the unit cell structural amplitude: $\boldsymbol{F_{HKL}}$

$$\boldsymbol{F_{HKL}} = \frac{\text{Coherent diffraction wave amplitude of a unit cell}}{\text{Coherently diffracted wave amplitude of an electron}} \qquad F_{HKL} = A_b / A_e = \sum_{j=1}^{n} f_j e^{i\phi_j}$$

We expand a complex number into trigonometric form

$$F_{HKL} = \sum_{j=1}^{n} f_j [\cos 2\pi(Hx_j + Ky_j + Lz_j) + i \sin 2\pi(Hx_j + Ky_j + Lz_j)]$$

The intensity of the X-rays $\boldsymbol{I_{HKL}}$ is proportional to the square of the structural amplitude $|\boldsymbol{F_{HKL}}|^2$

$$\left|F_{HKL}\right|^2 = F_{HKL} F_{HKL}^*$$

$|\boldsymbol{F_{HKL}}|^2$ is called structural factor. It is used to characterize the influence of the type, number and position of atoms in the unit cell on the (***H K L***) crystal plane diffraction intensity.

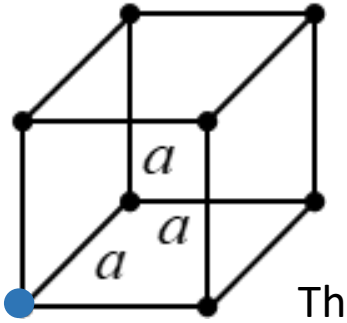
3.2 X-ray Scattering and Structure Factor of Unit Cell

Calculation of Lattice Structure Factors

$$F_{HKL} = \sum_{j=1}^{n} f_j[\cos 2\pi(Hx_j + Ky_j + Lz_j) + i \sin 2\pi(Hx_j + Ky_j + Lz_j)]$$

$$\left|F_{HKL}\right|^2 = F_{HKL} F_{HKL}^*$$

- Simple lattice



There is only one atom in the unit cell, its coordinates are (***H*** = 0,***K*** = 0, ***L*** = 0), and the atomic scattering factor is f, then we have:

$$|F_{HKL}|^2 = [f \cos 2\pi(0)]^2 + [f \sin 2\pi(0)]^2 = f^2$$

The structure factor of a simple lattice has nothing to do with ***H K L***, that is, if ***H K L*** is any integer, it can produce diffraction. For example: (100), (110), (111), (200), (210) …

If we define: $N_i = H_i^2 + K_i^2 + L_i^2$

Then the ratio of the sum of the squares of the interference surface index (***H K L***) that a simple lattice can produce diffraction is,

$(H_1^2 + K_1^2 + L_1^2) : (H_2^2 + K_2^2 + L_2^2) : (H_3^2 + K_3^2 + L_3^2)\ldots. = 1^2 : (1^2 + 1^2) : (1^2 + 1^2 + 1^2)\ldots. = 1:2:3:4:5..$

N_1 N_2 N_3

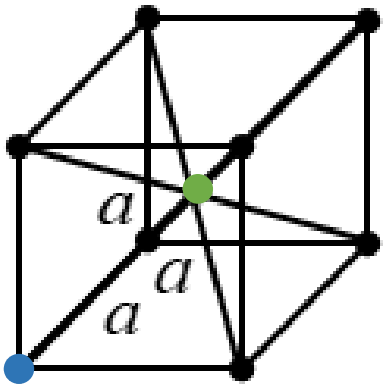
3.2 X-ray Scattering and Structure Factor of Unit Cell

Calculation of Lattice Structure Factors

$$\left|F_{HKL}\right|^2 = F_{HKL}F_{HKL}^*$$

$$F_{HKL} = \sum_{j=1}^{n} f_j[\cos 2\pi(Hx_j + Ky_j + Lz_j) + i\sin 2\pi(Hx_j + Ky_j + Lz_j)]$$

- Body-centered lattice



There are 2 atoms in the unit cell, the coordinates are (0,0,0) and (1/2,1/2,1/2), and the atomic scattering factors are ***f***.

$$|F_{HKL}|^2 = [f\cos 2\pi(0) + f\cos 2\pi(H+K+L)/2\,]^2 + [f\sin 2\pi(0) + f\sin 2\pi(H+K+L)/2\,]^2$$

$$= f^2[1+\cos\pi(H+K+L)]^2$$

1. When ***H*** + ***K*** + ***L***= odd numbers, $|F_{HKL}|^2 = \mathbf{0}$, diffraction intensity is zero. For instance, (100), (111), (210), (300), (311) …
2. When ***H*** + ***K*** + ***L***= even numbers, $|F_{HKL}|^2 = 4f^2$, these crystal planes can generate diffraction. For instance, (110), (200), (211), (310), … The ratio of the sum of squares of these interference plane indices (***H K L***) is:

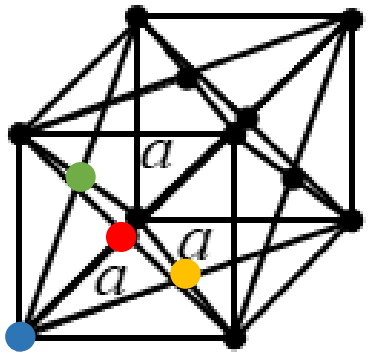
$$N_1 : N_2 : N_3 : N_4 : N_5 \cdots = 2:4:6:8:10\cdots$$

3.2 X-ray Scattering and Structure Factor of Unit Cell

Calculation of Lattice Structure Factors $\left|F_{HKL}\right|^2 = F_{HKL}F_{HKL}^*$

$$F_{HKL} = \sum_{j=1}^{n} f_j[\cos 2\pi(Hx_j + Ky_j + Lz_j) + i\sin 2\pi(Hx_j + Ky_j + Lz_j)]$$

- Face-centered lattice



There are 4 atoms in a unit cell. The coordinates are (0,0,0), (0,1/2,1/2) , (1/2, 0,1/2), (1/2,1/2, 0), and the atomic scattering factors are ***f***.

$$|F_{HKL}|^2 = f^2[1+\cos\pi(K+L)+\cos\pi(H+K)+\cos\pi(H+L)]^2$$

1. When ***H***, ***K***, ***L*** are odd and even mixed, $|F_{HKL}|^2 = \mathbf{0}$, diffraction intensity is zero. For instance, (100), (110), (210), (300), …
2. When ***H***, ***K***, ***L*** are all odd or all even numbers, $|F_{HKL}|^2 = \mathbf{16}f^2$, these crystal planes can generate diffraction. The ratio of the sum of squares of these interference plane indices (***H K L***) is:

$$N_1 : N_2 : N_3 : N_4 : N_5 \cdots = 3:4:8:11:12\cdots$$

3.2 X-ray Scattering and Structure Factor of Unit Cell

Diffraction surface index that can and cannot be diffracted in the lattice cell

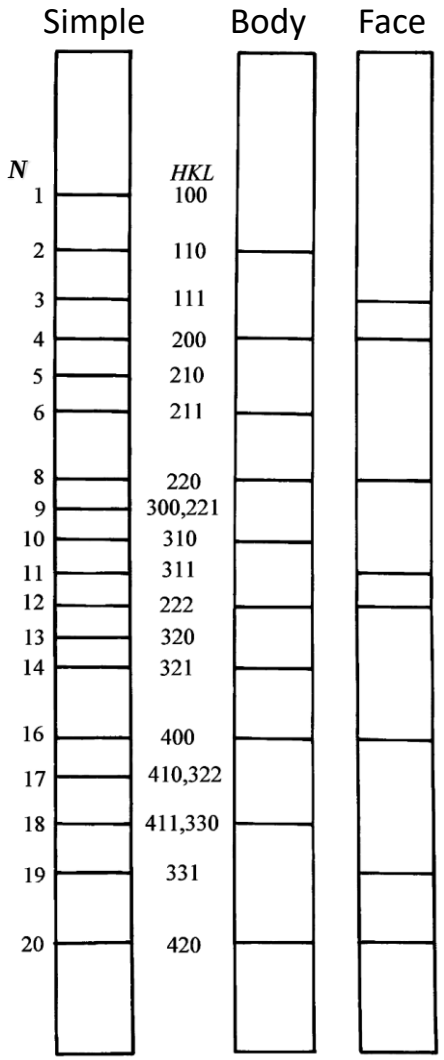
Lattice type	Diffraction prohibited (HKL)	Diffraction （HKL)	Structure factor
Simple	N/A	All	f^2
Base-centered	?	?	?
Body-centered	H + K + L = odd	H + K + L = even	$4f^2$
Face-centered	H、K、L odd and even mixed	H、K、L all odd or all even	$16f^2$

Only apply to single-element crystals

3.2 X-ray Scattering and Structure Factor of Unit Cell

The structure factor is only related to the type, number and position of the atoms in the unit cell and is not affected by the shape and size of unit cell.

The distribution of diffraction lines of three lattice crystals is shown in the figure.



The ratios of the sum of the square indices of the interference surface that produce diffraction are:
($N = H^2 + K^2 + L^2$)

Simple lattice **1 : 2 : 3 : 4 : 5 …**

Body-centered lattice **2 : 4 : 6 : 8 : 10 …**

Face-centered lattice **3 : 4 : 8 : 11 : 12 …**

3.2 X-ray Scattering and Structure Factor of Unit Cell

Matter composed of heterogeneous atoms

Substances composed of heterogeneous atoms, such as compound **AB**, belong to a simple lattice. **A** and **B** atoms occupy the top corners and centers of the unit cell respectively. Each of the two atoms forms a simple lattice. Its structure factors $|F_{HKL}|^2$ are:

1. When $H + K + L$ = odd number, $|F_{HKL}|^2 = (f_A - f_B)^2$
2. When $H + K + L$ = even number, $|F_{HKL}|^2 = (f_A + f_B)^2$

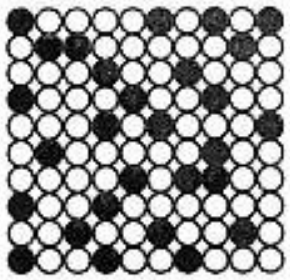
For the compound CuBe, due to the large difference in atomic numbers between Cu and Be, the diffraction line distribution is basically the same as that of a simple lattice.

CuZn has the same structure as CuBe, but because the atomic numbers of Cu and Zn are adjacent, f_{Cu} and f_{Zn} are very close, so their diffraction line distribution is the same as the body-centered lattice.

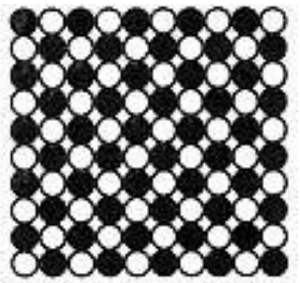
3.2 X-ray Scattering and Structure Factor of Unit Cell

Ordered solid solution

After an ordered transformation occurs in some solid solutions, different atoms will occupy specific positions in the unit cell, which will cause the diffraction line distribution to change accordingly.



Disordered



Ordered

For example, when $AuCu_3$ is a disordered solid solution, the extinction law follows the face-centered lattice;
In the ordered state, Au atoms occupy the vertex corners and Cu atoms occupy the face center. The result is:

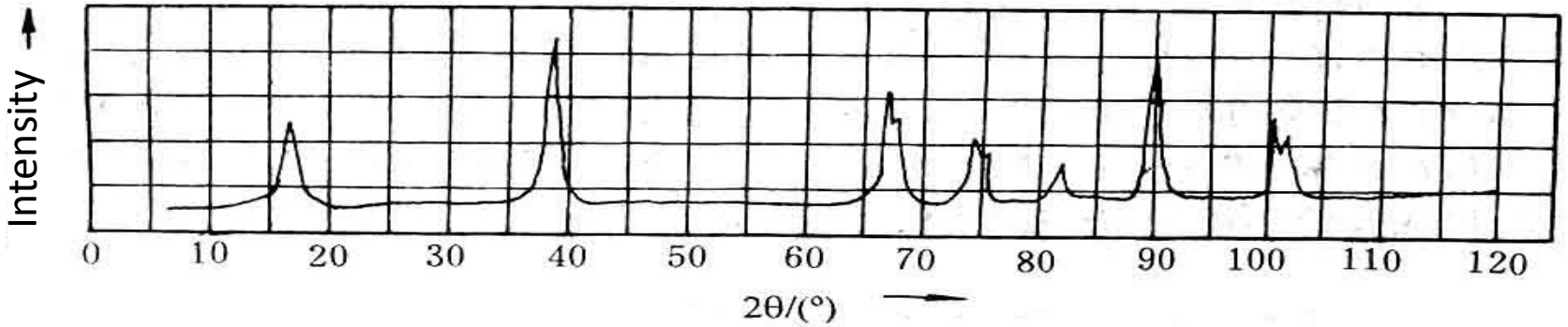
When ***H***, ***K***, ***L*** are odd and even mixed, $|F_{HKL}|^2 = (f_{Au} - f_{Cu})^2 \neq 0$

When ***H***, ***K***, ***L*** are all odd or even, $|F_{HKL}|^2 = (f_{Au} + 3f_{Cu})^2$

After the solid solution becomes ordered, the diffraction lines (lost by the disordered solid solution due to extinction) reappear.

3.3 Lorentz Factor

Integrated intensity of diffraction



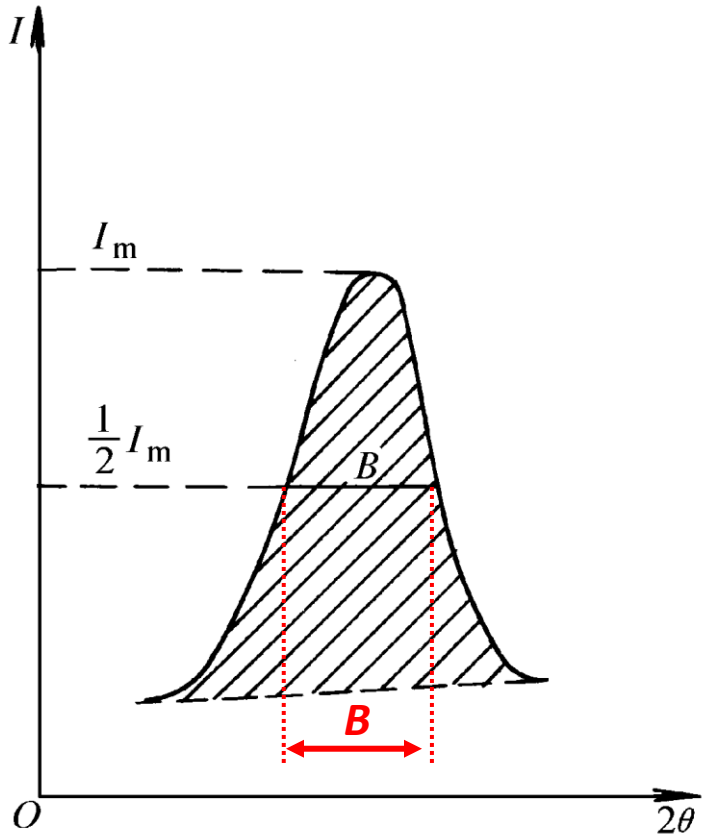
From the diffraction spectrum, the shape, height, and width of each diffraction peak are different. These diffraction peaks are related to the intensity of the diffraction line, but these phenomena cannot be explained by simply using the intensity. There are several main phenomena in the experiment:

1. When the detector records the intensity of the diffraction ray, it is always completed within a period of time, and the intensity recorded by the detector has a time accumulation effect.
2. The common diffraction of the same crystal plane of many grains in a polycrystalline sample is the sum of the diffraction lines of different grains. These diffraction peaks have a “quantitative” accumulation effect.
3. In diffractology, in order to measure this accumulation effect, a new concept is introduced—Integrated intensity of diffraction.

3.3 Lorentz Factor

Integrated intensity of diffraction

The diffraction integrated intensity is the area enclosed by the distribution curve (diffraction peak), which is called the diffraction integrated intensity.

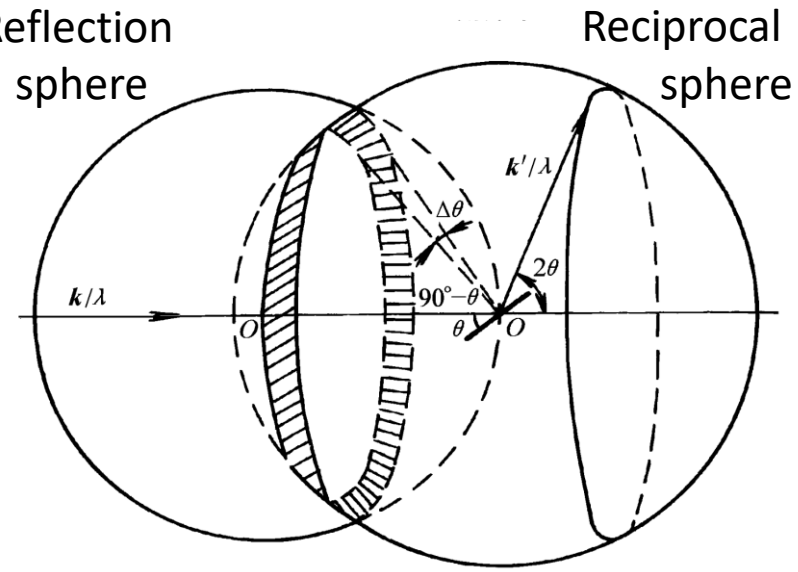


The diffraction integrated intensity is approximately equal to I_mB, I_m is the peak intensity, and B is the diffraction peak width at $I_m/2$ (called half-maximum width)

I_m is proportional to 1/sinθ, B is proportional to 1/cosθ, so the diffraction integrated intensity is proportional to 1/(sinθcosθ), that is, $1/\sin 2\theta$).

3.3 Lorentz Factor

Grain fraction participating in diffraction



The reciprocal points of (***H K L***) of the irradiated polycrystalline sample with random orientation distribution are uniformly distributed on the reciprocal sphere. The reciprocal points in the area of the reciprocal sphere ring (shadow) correspond to crystal planes to participate in the diffraction, that is, the ratio of the area of the ring to the area of the reciprocal sphere is the fraction of grains participating in the diffraction, which is proportional to ***cosϑ***.

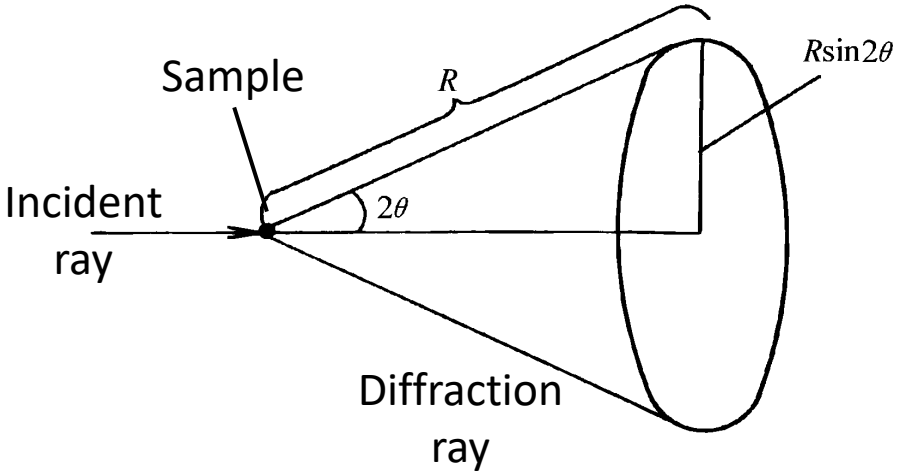
Fraction of grains participating in diffraction

$$= \frac{2\pi r^* \sin(90^\circ - \theta) r^* \Delta\theta}{4\pi (r^*)^2} = \frac{\cos\theta}{2}\Delta\theta$$

In the equation, ***r**** is the radius of the reciprocal sphere, ***r***Δθ*** is the ring width.

3.3 Lorentz Factor

Diffraction intensity per unit arc length



On a diffraction ring with a diffraction angle of ***2ϑ***, the distance from a certain point to the sample is **R,** then the radius of the diffraction ring is ***Rsin2ϑ*** and the perimeter is ***2πRsin2ϑ***.

It can be seen that the diffraction intensity per unit arc length is proportional to ***1/sin2ϑ***.

Lorentz factor
- Integrated intensity of diffraction (**1/sin2θ**)
- Grain fraction participating in diffraction (**Cosθ**)
- Diffraction intensity per unit arc length (**1/sin2θ**)

$$\frac{1}{\sin 2\theta}\cos\theta\frac{1}{\sin 2\theta} = \frac{1}{4\sin 2\theta\cos\theta}$$

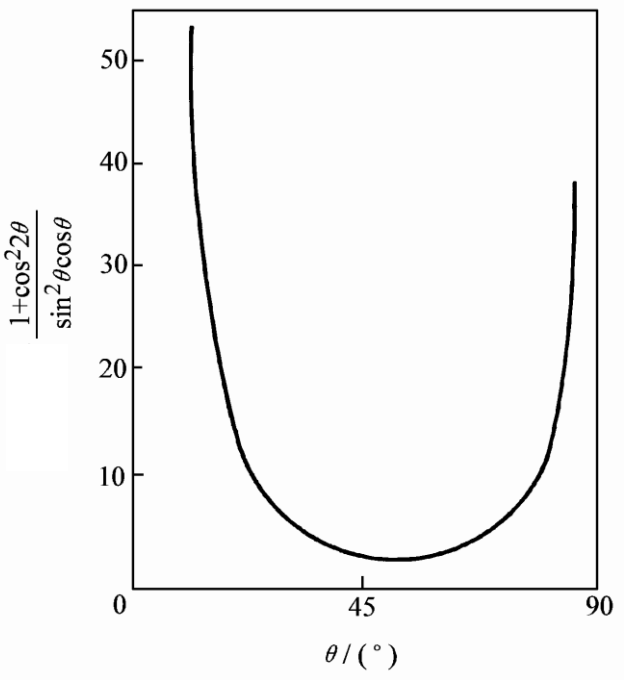
3.3 Lorentz Factor

Angle factor

Combining the Lorentz factor with the polarization factor, a function related to the glancing angle θ can be obtained, called the angle factor, or the Lorentz-polarization factor

$$\text{Lorentz factor} = \frac{1}{4\sin 2\theta \cos\theta} \qquad \text{Polarization factor} = \frac{1+(\cos 2\theta)^2}{2}$$

$$\text{Angle factor} = \frac{1+\cos^2 2\theta}{8\sin^2\theta\cos\theta}$$



The angle factor changes with θ as shown in the figure.

3.4 Other factors that influence diffraction intensity

Multiplicity Factor (**P**)

The crystal planes of the same crystal plane group {***h k l***} in the crystal have the same atomic arrangement and equal crystal plane spacing ***d***, so their diffraction angles 2θ are the same. In the polycrystal diffraction pattern, their diffraction will overlap in the same diffraction ring.

As the number of equivalent crystal planes increases, the probability of participating in diffraction increases, and the corresponding diffraction intensity will also increase.

The effect of the equivalent number of crystal planes on the diffraction intensity is called the multiplicity factor **P**, and the multiplicity factor is related to the symmetry of the crystal and the crystal plane index.

For example, the {100} plane family P =6 and {110} plane family P =12 of the cubic crystal system; the {100} plane family P =4 and {001} plane family P =2 of the tetragonal crystal system.

3.4 Other factors that influence diffraction intensity

Multiplicity Factor (**P**)

According to the Bragg equation ***2d sinϑ= λ***, when ***λ*** is constant, the diffraction rays of all the diffraction plane with the same interplanar spacing overlap into one. The diffraction intensity is the sum of the intensity of these plane diffraction rays.

Example: cubic crystal system: $$d=\frac{a}{\sqrt{H^2+K^2+L^2}}$$

For the {***1 0 0***} crystal plane family: there are 6 crystal planes:

(100) (010) (001) $(\bar{1}00)$ $(0\bar{1}0)$ $(00\bar{1})$ ***d*** same **P** = 6

Example: tetragonal crystal system: $$d=\frac{1}{\sqrt{\frac{H^2+K^2}{a^2}+\frac{L^2}{c^2}}}$$

For the {***1 0 0***} crystal plane family: there are 4 crystal planes:

(100) (010) $(\bar{1}00)$ $(0\bar{1}0)$ ***d*** same **P** = 4

For the {***0 0 1***} crystal plane family: (001) $(00\bar{1})$ ***d*** same **P** = 2

3.4 Other factors that influence diffraction intensity

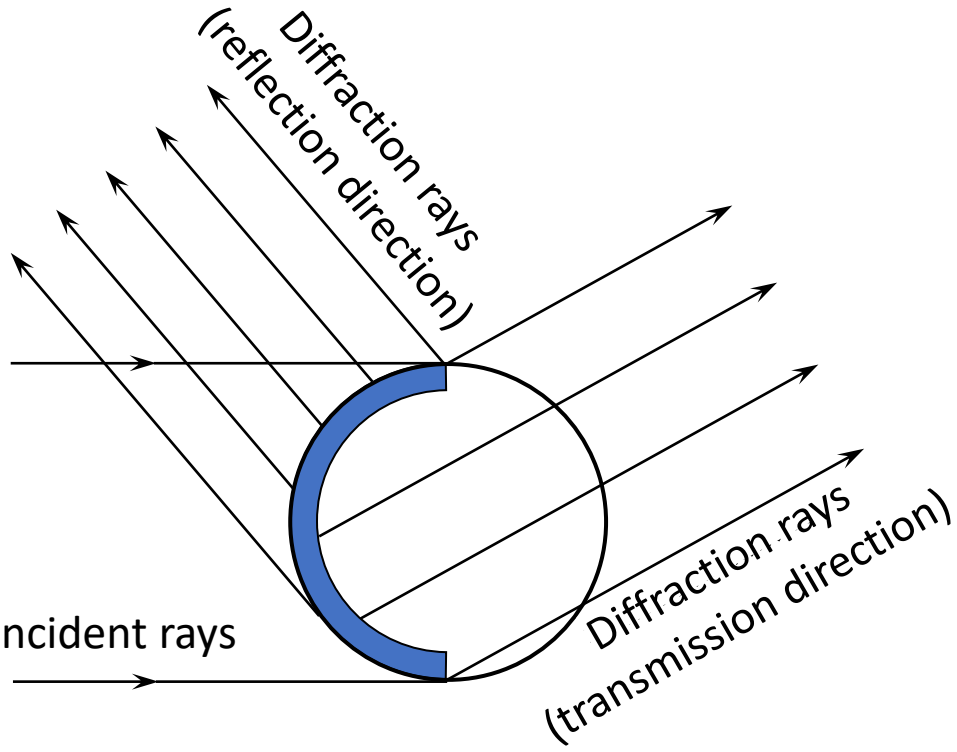
Multiplicity Factor (**P**)

	H00	0k0	00L	HHH	HH0	HK0	0KL	H0L	HHL	HKL
Cubic	**6**			**8**	**12**	**24***			**24**	**48***
Hexagonal Trigonal	**6**		**2**		**6**	**12***	**12***		**12***	**24***
Tetragonal	**4**		**2**		**4**	**8***	**8**		**8**	**16***
Orthorhombic	**2**	**2**	**2**			**4**	**4**	**4**		**8**
Monoclinic	**2**	**2**	**2**			**4**	**4**	**2**		**4**
Triclinic	**2**	**2**	**2**			**2**	**2**	**2**		**2**

3.4 Other factors that influence diffraction intensity

Absorption Factor

Due to the absorption of X-rays by the sample itself, the actual measured value of the diffraction intensity does not match the calculated value, so the intensity needs to be corrected by the absorption factor $A(\theta)$. The absorption factor $A(\theta)$ is related to the shape, size, composition and diffraction angle of the sample.



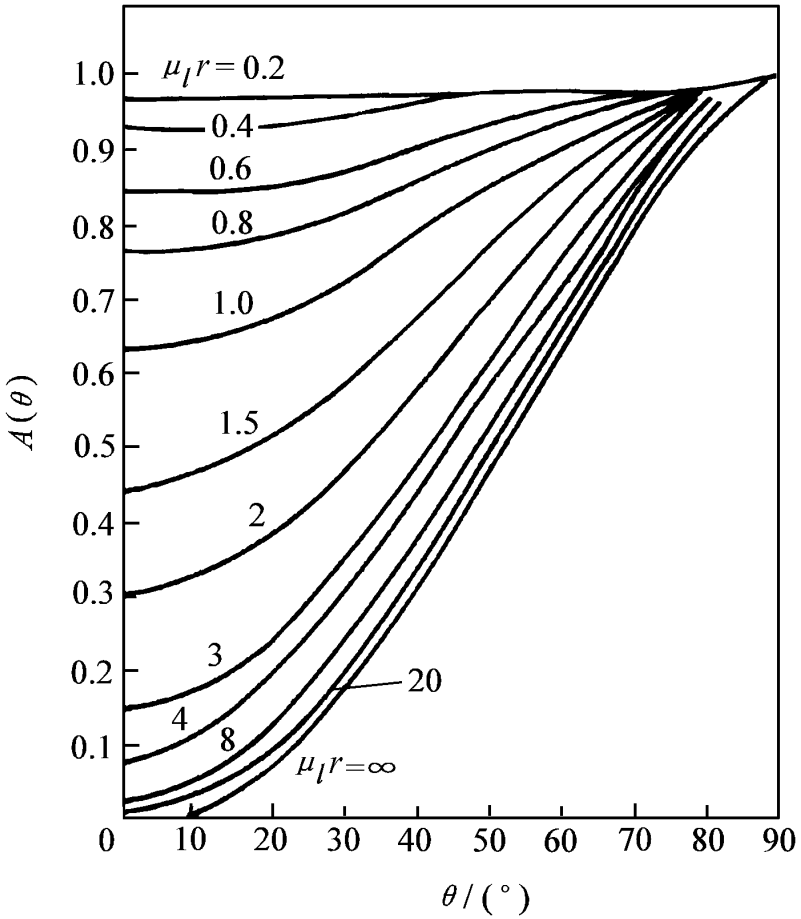
1. Cylindrical specimen

When the specimen radius r and line absorption coefficient μ_l are large, only the thin layer of material on the surface participates in diffraction. Diffraction rays passing through the sample are also absorbed. The absorption in the transmission direction is more serious, while the reflection direction has less impact.

3.4 Other factors that influence diffraction intensity

Absorption Factor

1. Cylindrical specimen



For the same sample, the larger the **θ**, the smaller the absorption; in the same **θ** direction, the larger the $\mu_l r$, the smaller the $A(\theta)$ is, and the change of $A(\theta)$ with $\mu_l r$ and **θ** is shown in the figure.

When the diffraction intensity is not affected by absorption, take $A(\theta)$ = 1.

The absorption factor of the cylindrical specimen can be found in relevant information.

3.4 Other factors that influence diffraction intensity

Absorption Factor

2. Flat Specimen

The X-ray diffractometer uses a flat sample, and its absorption factor has approximately nothing to do with **θ**, but is inversely proportional to μ_l , that is

$$A(\theta) = 1/2\mu_l$$

3.4 Other factors that influence diffraction intensity

Temperature Factor

The thermal vibration of atoms worsens the periodicity of the atomic arrangement in the lattice, causing the coherent scattering that strictly satisfies the Bragg condition to generate additional phase differences, thereby weakening the diffraction intensity.

The temperature factor e^{-2M} is introduced into the diffraction intensity formula, which is the ratio of the diffraction intensity at temperature T to the diffraction intensity at 0K, that is, $I_T / I = e^{-2M}$, which can be derived from solid state physics.

$$M = \frac{6h^2}{m_a k\Theta}\left[\frac{\phi(x)}{x} + \frac{1}{4}\right]\frac{\sin^2\theta}{\lambda^2}$$

In the formula, h is Planck's constant; m_a is atomic weight; k is Boltzmann's constant; Θ is the average value of crystal characteristic temperature represented by thermodynamic temperature; $x = \Theta/T$, T is the thermodynamic temperature; $\phi(x)$ is the Debye function.

3.4 Other factors that influence diffraction intensity

Temperature Factor

- The higher the sample temperature ***T***, the smaller x, the more violent the atomic thermal vibration, and the lower the diffraction intensity.
- When the sample temperature T is constant, the larger the glancing angle **θ**, the smaller the e^{-2M}, and the lower the diffraction intensity.
- For cylindrical specimens, when **θ** changes, the temperature factor and absorption factor have opposite trends, and their effects can be roughly offset. For analysis with less precise strength requirements, e^{-2M} and $A(\theta)$ can be ignored at the same time.
- The thermal vibration of atoms not only weakens the diffraction intensity, but also increases the background intensity of the diffraction, and it becomes more serious as the θ angle increases.

3.5 Integral intensity formula for polycrystalline diffraction

Factors of Integrated intensity of diffraction

- Structure factor ⋯⋯▸ $\left|F_{HKL}\right|^2$
- Angle factor ⋯⋯▸ $\dfrac{1+\cos^2 2\theta}{8\sin^2\theta\cos\theta}$
- Multiplicity factor ⋯⋯▸ P
- Absorption factor ⋯⋯▸ $A(\theta)$
- Temperature factor ⋯⋯▸ e^{-2M}

3.5 Integral intensity formula for polycrystalline diffraction

If X-rays with wavelength $\boldsymbol{\lambda}$ and intensity $\boldsymbol{I_0}$ are irradiated onto a polycrystalline sample with unit cell volume $\boldsymbol{V_0}$, and the irradiated volume is $\boldsymbol{V}$, (***H K L***) diffraction will occur in the **2θ** direction, The recorded diffraction integrated intensity (at a distance ***R*** from the sample) is:

$$I = I_0 \frac{\lambda^3}{32\pi R}\left(\frac{e^2}{mc^2}\right)\frac{V}{V_0^2} P\left|F_{HKL}\right|^2 \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta} A(\theta)e^{-2M}$$

The result of the above formula is the absolute integral intensity, and the actual application generally only needs to consider the relative value. For each diffraction line of the same phase in the same diffraction pattern, the first four terms of the above formula can be regarded as constants, so the relative integral intensity of the diffraction line is:

$$I_{Relative} = P\left|F_{HKL}\right|^2 \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta} A(\theta)e^{-2M}$$

If you compare the diffraction of different phases in the same diffraction pattern, you still need to consider the irradiated volume of each phase and the unit cell volume of each phase.